Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssptansc1625

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

=>

Uploading C:\Program Files\Stnexp\Queries\10507925C.str

16 15 15 18 11 11

chain nodes:
10 11 12 15 16
ring nodes:
1 2 3 4 5 6 7 8 9
chain bonds:
6-15 10-11 11-12 15-16
ring bonds:
1-2 1-6 2-3 3-4 3-7 4-5 4-9 5-6 7-8 8-9
exact/norm bonds:
3-7 4-9 7-8 8-9 10-11 11-12 15-16
exact bonds:
6-15 normalized bonds:
1-2 1-6 2-3 3-4 4-5 5-6

G1:0,S,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 15:CLASS 16:CLASS 18:Atom

=> D L5 L5 HAS NO ANSWERS 1.5 STR

Structure attributes must be viewed using STN Express query preparation.

1 ANSWERS

=> S SSS L5 SAM SAMPLE SEARCH INITIATED 18:58:39 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 14700 TO ITERATE

13.6% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE** BATCH **COMPLETE**

PROJECTED ITERATIONS: 286737 TO 301263 PROJECTED ANSWERS: 1 TO 309

1 SEA SSS SAM L5 L6

=> D SCAN

L6 1 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN Ethanone, 1-[6-hydroxy-4-methoxy-7-(3-phenoxypropoxy)-5-benzofuranyl]-C20 H20 O6 MF

ALL ANSWERS HAVE BEEN SCANNED

=> S SSS L5 FULL

FULL SEARCH INITIATED 18:58:53 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 292385 TO ITERATE

100.0% PROCESSED 292385 ITERATIONS

125 ANSWERS

SEARCH TIME: 00.00.02

L7 125 SEA SSS FUL L5

=> D SCAN

L7 125 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN Acetic acid, [[4,7-dimethoxy-5-[1-oxo-3-(3,4,5-trimethoxyphenyl)-2-

propenyl]-6-benzofuranyl]oxy]- (9CI)

MF C24 H24 O10

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ENTER NAME OR (END): END

=> SAVE TEMP L7 BAEL10507925/A
ANSWER SET L7 HAS BEEN SAVED AS 'BAEL10507925/A'

_.

Uploading C:\Program Files\Stnexp\Queries\10507925D.str

chain nodes : 10 11 12 15 16 27 28

ring nodes:
1 2 3 4 5 6 7 8 9 18 19 20 21 22 23 24 25 26

chain bonds:

1-10 6-15 10-11 11-12 12-18 15-16 19-27 27-28

ring bonds:

1-2 1-6 2-3 3-4 3-7 4-5 4-9 5-6 7-8 8-9 18-19 18-23 19-20 20-21 21-22

21-24 22-23 22-26 24-25 25-26

exact/norm bonds:

1-10 3-7 4-9 7-8 8-9 10-11 11-12 12-18 15-16 21-24 22-26 24-25 25-26

exact bonds:

8xact bonds:

6-15 19-27 normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 18-19 18-23 19-20 20-21 21-22 22-23

G1:0,S,N

Match level: 1:1Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 15:CLASS 16:CLASS 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 27:CLASS 28:CLASS

L8 STRUCTURE UPLOADED

=> D L8 L8 HAS NO ANSWERS L8 STR

Structure attributes must be viewed using STN Express query preparation.

=> S SSS L8 SAM
SAMPLE SEARCH INITIATED 19:05:47 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 94 TO ITERATE

100.0% PROCESSED 94 ITERATIONS 0 ANSWERS SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE** BATCH **COMPLETE** PROJECTED ITERATIONS: 1299 TO 2461

PROJECTED ANSWERS: 0 TO 0

L9 0 SEA SSS SAM L8

=> S SSS L8 SUBSET=L7 SAM
SAMPLE SUBSET SEARCH INITIATED 19:06:23 FILE 'REGISTRY'
SAMPLE SUBSET SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

PROJECTIONS (WITHIN SPECIFIED SUBSET): ONLINE **COMPLETE**
PROJECTED ITERATIONS (WITHIN SPECIFIED SUBSET): 0 TO 0
PROJECTED ANSWERS (WITHIN SPECIFIED SUBSET): 0 TO 0

L10 0 SEA SUB=L7 SSS SAM L8

=> D SCAN L10 HAS NO ANSWERS

=>

Uploading C:\Program Files\Stnexp\Queries\10507925E.str

ring nodes:
1 2 3 4 5 6 7 8 9 18 19 20 21 22 23 24 25 26
chain bonds:
1-10 6-15 10-11 11-12 12-18 15-16 19-27 27-28
ring bonds:
1-2 1-6 2-3 3-4 3-7 4-5 4-9 5-6 7-8 8-9 18-19 18-23 19-20 20-21 21-22
21-24 22-23 22-26 24-25 25-26
exact/norm bonds:
1-10 3-7 4-9 7-8 8-9 10-11 11-12 12-18 15-16 21-24 22-26 24-25 25-26
exact bonds:
exact bonds:
exact bonds:
6-15 19-27

normalized bonds :

chain nodes :

10 11 12 15 16 27 28

 $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 18-19 \quad 18-23 \quad 19-20 \quad 20-21 \quad 21-22 \quad 22-23$

G1:0,S,N

Match level: 1:Atcm 2:Atcm 3:Atcm 4:Atcm 5:Atcm 6:Atcm 7:Atcm 8:Atcm 9:Atcm 10:CLASS 11:CLASS 12:CLASS 15:CLASS 16:CLASS 18:Atcm 19:Atcm 20:Atcm 21:Atcm 22:Atcm 2:Atcm 2:4Atcm

L11 STRUCTURE UPLOADED

=> D L11

L11 HAS NO ANSWERS L11 STR

Structure attributes must be viewed using STN Express query preparation.

0 TO

=> S SSS L11 SAM

SAMPLE SEARCH INITIATED 19:08:16 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 112 TO ITERATE

100.0% PROCESSED 112 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE** PROJECTED ITERATIONS: 1606 TO 2874 PROJECTED ANSWERS:

L12 0 SEA SSS SAM L11

=> D HIS

1.10

(FILE 'HOME' ENTERED AT 18:40:49 ON 11 MAR 2008)

FILE 'REGISTRY' ENTERED AT 18:41:03 ON 11 MAR 2008 L1 STRUCTURE UPLOADED L2 1 S SSS L1 SAM L3 STRUCTURE UPLOADED L4 1 S SSS L3 SAM L5 STRUCTURE UPLOADED 1 S SSS L5 SAM L6 125 S SSS L5 FULL SAVE TEMP L7 BAEL10507925/A 1.8 STRUCTURE UPLOADED 0 S SSS L8 SAM L9

0 S SSS L8 SAM SUB=L7

L11 STRUCTURE UPLOADED L12 0 S SSS L11 SAM

=> S SSS L11 SUBSET=L7 SAM

SAMPLE SUBSET SEARCH INITIATED 19:09:07 FILE 'REGISTRY'
SAMPLE SUBSET SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

PROJECTIONS (WITHIN SPECIFIED SUBSET): ONLINE **COMPLETE**
PROJECTED ITERATIONS (WITHIN SPECIFIED SUBSET): 0 TO 0
PROJECTED ANSWERS (WITHIN SPECIFIED SUBSET): 0 TO 0

L13 0 SEA SUB=L7 SSS SAM L11

=>

=> S SSS L11 SUBSET=L7 FULL FULL SUBSET SEARCH INITIATED 19:09:24 FILE 'REGISTRY' FULL SUBSET SCREEN SEARCH COMPLETED - 17 TO ITERATE

100.0% PROCESSED 17 ITERATIONS 5 ANSWERS

SEARCH TIME: 00.00.01

L14 5 SEA SUB=L7 SSS FUL L11

=> FIL CAPL

 COST IN U.S. DOLLARS
 SINCE FILE
 TOTAL

 ENTRY
 SESSION

 FULL ESTIMATED COST
 241.62
 241.83

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=> S L14

L15 4 L14

=> D IBIB ABS HITSTR 1-4

L15 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2006:87666 CAPLUS Full-text

DOCUMENT NUMBER: 144:331145

TITLE: A New Class of Blockers of the Voltage-Gated Potassium Channel Kv1.3 via Modification of the 4- or 7-Position of Khellinone

AUTHOR(S): Harvey, Andrew J.; Baell, Jonathan B.; Toovey, Nathan;

Homerick, Daniel; Wulff, Heike

CORPORATE SOURCE: The Walter and Eliza Hall Institute, Medical Research

Biotechnology Centre, Bundoora, 3086, Australia Journal of Medicinal Chemistry (2006), 49(4),

1433-1441

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

LANGUAGE: English

OTHER SOURCE(S): CASREACT 144:331145

AB The voltage-gated potassium channel Kv1.3 constitutes an attractive target for the selective suppression of effector memory T cells in autoimmune diseases.

We have previously reported the natural product khellinone, as a versatile lead mol. and identified two new classes of KV1.3 blockers: (i) chalcone derivs. of khellinone, and (ii) khellinone dimers linked through the 6-position. Here we describe the multiple parallel synthesis of a new class of khellinone derivs. selectively alkylated at either the 4- or 7-position via the phenolic OH and show that several chloro, bromo, methoxy, and nitro substituted benzyl derivs. inhibit KV1.3 with submicromolar potencies. Representative examples of the most potent compds. from each subclass, (5-acetyl-4-(4"chloro)benzyloxy-6-hydroxy-7- methoxybenzofuran) and (5-acetyl-7-

Representative examples of the most potent compds. from each subclass, (5-acetyl-4-(4'-chloro)benzyloxy-6-hydroxy-7-methoxybenzofuran) and (5-acetyl-7-(4'-bromo)benzyloxy-6-hydroxy-4-methoxybenzofuran), block Kv1.3 with EC50 values of 480 and 400 nM, resp. Both compds. exhibit moderate selectivity over other Kv1-family channels and HERG, are not cytotoxic, and suppress human T

cell proliferation at low micromolar concns.

IT 880479-06-1P

SOURCE:

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and voltage-gated potassium channel activity of khellinone analogs)

RN 880479-06-1 CAPLUS

CN Ethanone, 1,1'-[1,6-hexanediylbis[oxy(4-ethoxy-7-methoxy-6,5-

benzofurandiyl)]]bis- (9CI) (CA INDEX NAME)

REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2004:446728 CAPLUS Full-text DOCUMENT NUMBER: 141:251728

TITLE: 1,6-Bis(5-acetyl-4,7-dimethoxybenzofuran-6-

yloxy)hexane

AUTHOR(S): Baell, Jonathan B.; Gable, Robert W.; Harvey, Andrew

J.

CORPORATE SOURCE: Structural Biology Chemistry Group, The Walter and

Eliza Hall Institute of Medical Research, Biotechnology Centre, Bundoora, Victoria, 3086,

Australia

SOURCE: Acta Crystallographica, Section E: Structure Reports

Online (2004), E60(6), o996-o997 CODEN: ACSEBH: ISSN: 1600-5368

PUBLISHER: International Union of Crystallography

DOCUMENT TYPE: Journal; (online computer file)

LANGUAGE: English

AB The khellinone dimer, 1,6-bis-(5-acetyl-4,7-dimethoxybenzofuran-6yloxy)hexane, C30H34010, was prepared as part of Kv1.3 ion channel blockers. Crystallog, data are given. The dimer lies on a center of symmetry, and

trystallog, data are given. The dimer fles on a center or symmetry, adopts an extended structure such that the separation between the benzofuran groups is 9.927(3) Å. C-H···O H bonds link the mols. into linear chains which lie parallel to the [201] direction.

IT 605665-31-4P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(preparation and crystal structure of)

RN 605665-31-4 CAPLUS

CN Ethanone, 1,1'-[1,6-hexanediylbis[oxy(4,7-dimethoxy-6,5-

benzofurandiyl)]]bis- (9CI) (CA INDEX NAME)

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2004:178993 CAPLUS Full-text

DOCUMENT NUMBER: 140:375004

TITLE: Khellinone Derivatives as Blockers of the

Voltage-Gated Potassium Channel Kv1.3: Synthesis and

Immunosuppressive Activity

AUTHOR(S): Baell, Jonathan B.; Gable, Robert W.; Harvey, Andrew

J.; Toovey, Nathan; Herzog, Tanja; Haensel, Wolfram;

Wulff, Heike

CORPORATE SOURCE: Walter and Eliza Hall Institute of Medical Research
Biotechnology Centre, Bundoora, 3086, Australia

SOURCE: Journal of Medicinal Chemistry (2004), 47(9),

2326-2336

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:375004

AB The voltage-gated potassium channel Kv1.3 constitutes a promising new target for the treatment of T-cell-mediated autoimmune diseases such as multiple sclerosis. In this study, we report the discovery of two new classes of Kv1.3 blockers based on the naturally occurring compound khellinone, 5-acetyl-4,7-

dimethoxy-6-hydroxybenzofuran: (1) khellinone dimers linked via the alkylation of the 6-hydroxy groups and (2) chalcone derivs. of khellinone formed by Claisen-Schmidt condensation of the 5-acetyl group with aryl aldehydes. In particular, the chalcone 3-(4,7-dimethoxy-6-hydroxybenzofuran-5-yl)-1-phenyl-3-oxopropene and several of its derivs. inhibited Kul.3 with Kd values of 300-800 nM and a Hill coefficient of 2, displayed moderate selectivity over other KVI-family K+ channels, suppressed T-lymphocyte proliferation at submicromolar concas., and showed no signs of acute toxicity in mice. Because of their relatively low mol. weight and lipophilicity and their high affinity to KVI.3, aryl-substituted khellinone derivs. represent attractive lead compds. for the development of more potent and selective KVI.3 blocking immunosuppressants.

IT 605665-30-3P 605665-31-4P 605665-32-5P 684278-39-5P

RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and immunosuppressive activity of khellinone derivs.)
RN 605665-30-3 CAPLUS

CN Ethanone, 1,1'-[1,5-pentanediylbis[oxy(4,7-dimethoxy-6,5-benzofurandiyl]]bis- (9CI) (CA INDEX NAME)

RN 605665-31-4 CAPLUS

CN Ethanone, 1,1'-[1,6-hexanediylbis[oxy(4,7-dimethoxy-6,5-benzofurandiyl)]]bis- (9CI) (CA INDEX NAME)

RN 605665-32-5 CAPLUS

CN Ethanone, 1,1'-[1,4-butanediylbis[oxy(4,7-dimethoxy-6,5-benzofurandiyl)]]bis- (9CI) (CA INDEX NAME)

REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD, ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2003:757693 CAPLUS Full-text

DOCUMENT NUMBER: 139:276752

TITLE: Preparation of divalent ligands based on khellinone derivatives as therapeutic ion channel blocking agents

INVENTOR(S): Baell, Jonathan B.; Wulff, Heike; Harvey, Andrew J.; Norton, Raymond S.; Chandy, George K.

PATENT ASSIGNEE(S): The Walter and Eliza Hall Institute of Medical

Research, Australia SOURCE: PCT Int. Appl., 64 pp.

CODEN: PIXXD2 DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

PATENT NO. KIND APPLICATION NO. DATE DATE WO 2003078416 A1 20030925 WO 2003-AU351 20030320 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GO, GW, ML, MR, NE, SN, TD, TG CA 2479481 A1 20030925 CA 2003-2479481 20030320 AU 2003212101 20030929 AU 2003-212101 A1 20030320 EP 1490349 EP 2003-707912 A1 20041229 20030320 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK CN 1656087 20050817 CN 2003-811505 20030320 A JP 2005525384 20050825 JP 2003-576422 20030320 IN 2004DN02795 Α 20070420 IN 2004-DN2795 20040920 A1 US 2005261301 20051124 US 2005-507925 20050705 PRIORITY APPLN. INFO.: AU 2002-1272 A 20020320 WO 2003-AU351 W 20030320

OTHER SOURCE(S): MARPAT 139:276752

GI

AB The title compds. II, R1-R4 = H, OH, alkyl, alkoxy, etc., X = a divalent spacer group that provides a spacing between the two aromatic rings to which it is joined of from 6 to 11 atoms when measured across the shortest route between the two aromatic rings; A, B = fused rings independently selected from (un)substituted 5-7 membered (hetero) aromatic and non-aromatic heterocyclic rings; R5, R6 = COR7, C(NR7)R7, CSR7 (R7 = H, alkyl, alkoxy, OH); with the proviso) which can be useful in the modulation of potassium channel activity in cells, including among others Kvl.3 channels found in T-cells, were prepared Thus, reacting khellinone with 1,5-dibromopentane in the presence of cesium carbonate in DMF afforded 65% II which showed Kd of 0.82 µM (Kvl.3) and Kd of 1.5 µM (Kvl.2). The compds. I may also be useful in the treatment or prevention of autoimmune and inflammatory diseases, including multiple sclerosis. Pharmaceutical composition comprising the compound I was claimed. 10 05065-3-0-3 Pc 05065-3-1-3-5-5

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(preparation of divalent ligands based on khellinone derivs. as therapeutic ion channel blocking agents)

RN 605665-30-3 CAPLUS

CN Ethanone, 1,1'-[1,5-pentanediylbis[oxy(4,7-dimethoxy-6,5-benzofurandiyl]]bis-(9CI) (CA INDEX NAME)

RN 605665-31-4 CAPLUS

CN Ethanone, 1,1'-[1,6-hexanediylbis[oxy(4,7-dimethoxy-6,5-benzofurandiyl)]]bis- (9CI) (CA INDEX NAME)

RN 605665-32-5 CAPLUS

CN

Ethanone, 1,1'-[1,4-butanediylbis[oxy(4,7-dimethoxy-6,5-benzofurandiyl)]]bis- (9CI) (CA INDEX NAME)

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> LOGOFF H

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	25.64	267.47
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL
CA SUBSCRIBER PRICE	-3.20	-3.20

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FILE 'CAPLUS' ENTERED AT 19:14:46 ON 11 MAR 2008
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	ENTRY	SESSION
FULL ESTIMATED COST	25.64	267.47
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL

CA SUBSCRIBER PRICE	ENTRY -3.20	SESSION -3.20
=> =>		
=> LOGOFF Y COST IN U.S. DOLLARS FULL ESTIMATED COST	SINCE FILE ENTRY 26.60	TOTAL SESSION 268.43
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) CA SUBSCRIBER PRICE	SINCE FILE ENTRY -3.20	TOTAL SESSION -3.20

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